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Self-Improving Methods for Materials and Process Design

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1. Objective

This research is to develop a self-improving system that is capable of performing concept formation for associating materials and process design using inductive and deductive coupling techniques.

2. Status of Effort

The first phase of the work focuses on developing an artificial neural network learning for function approximation. The objective for neural network function approximation is to learn the input-output mapping efficiently. Different with traditional gradient descent-based search algorithm such as back-propagation and its variations, we have developed a rapid neural network unsupervised learning algorithm. Not only the learning algorithm can update the weights of the neural networks instantly for a newly added input, but also it can update the weight for a newly added neuron immediately. We have applied this algorithm and architecture to different applications, such as for the mapping and prediction of an infrared laser data set, a chaotic time-series, a monthly flour price data set, and identification of a non-linear system.

The second phase of the work focuses on developing an artificial neural network learning algorithm for time-series prediction. A dynamic stepwise updating algorithm is proposed to update the weight of the system in-situ. We also focus the work on regularization and development of functional space theory. It is well known that the goal of neural network function approximation is not to learn an exact representation of the training data, but rather to build a statistical model for smooth interpolation. In practical, if a network is over-fitting to the noise on the training data, it will give a poor generalization. To solve this problem, there are two main approaches: model selection and regularization. Model selection (the main focus of the third phase) for a feed-forward neural network requires choosing the number of hidden neurons and connection weights. The common statistical approach for model selection is to estimate the generalization error for each model and to choose a model with minimum error. While regularization approach involves

constraining or penalizing the solution of the estimation problem to improve network generalization ability by smoothing the predictions.

The third phase of the work focuses on model selection. We have successfully used both neural networks approach and neuro-fuzzy approach to select the most important features (attributes) for function mapping and construct a model with a minimum generalization error. We have applied this approach, successfully, identifying material properties and predicting ternary systems compounding formation.

3. Accomplishments/New Findings

3.1 Research Highlights and Contribution

The first phase work focuses on designing a new single-hidden layer artificial neural network architecture and an instant learning algorithm that rapidly decides its weights. Improving the learning speed of back-propagation (BP) and increasing the generalization capability of the networks have played a center role in neural network research. Apart from multi-layer network architectures and the as the BP algorithm, various simplified architectures or different non-linear activation functions have been devised. Among those, a so-called flat networks including functional-link neural network and radial basis function network have been proposed. These flat networks remove the drawback of a long learning process with the advantage of learning only one set of weights. Most importantly, the literature has reported satisfactory generalization capability in function approximation.

We have developed a one-step fast learning algorithm and a stepwise update algorithm for training the flat networks. The algorithms are developed based on the formulation of the network that has a set of linear system equations. The most significant advantage of the stepwise approach is that the weight connections of network can be updated easily, when a new input is given later after the network has been trained. The weights can be updated easily based on the original weights and the new inputs. The stepwise approach

also is able to update weights instantly when a new neuron is added to the existing network if the desired error criterion cannot be met. With this learning algorithm, the networks become very attractive in terms of learning speed.

The second phase focuses on the work of regularization and development of functional space theory. Combining our approach and unsupervised learning algorithm, we have extended the capability of discovery methods on materials research, such as predicting material properties. Our regularization approach combines orthogonal least square method and subset selection. The benefit of the research is to reduce number of regressors (neurons) in the functional mapping. If the network has too many regressors, it will cause the network to be overly sensitive to the training data, which often results in poor generalization. We have developed an orthogonal function transformation and an orthogonal functional basis neural network (OFBNN) based on this transformation. We have applied this approach to electro-optic (EO) data of several semiconductor compounds. The OFBNN model has been used to learn a function-related attribute of compounds, which form a “cluster” based on similar attribute values. We are able to learn the function and to predict the feature value of compounds in a cluster. The result of the EO data gives us a very promising result.

In the third phase of the work, the focus is on the model selection. We have applied neural networks and neuro-fuzzy hybrid model to explore materials and process discovery. We have successfully identified material properties that determine the internal structure of ternary system compounding forming. Our neural network learning algorithm suggests that one of the features, i.e., *Mendeleev number* dominates more than 90% of the accuracy of compound formation. Our neuro-fuzzy approach for model selection suggests that *Zunger difference*, *Energy difference*, *Average*, *Variance*, and *Ratio of Mendeleev number* play the most important role for the formation and for future prediction. This is the model with the minimum generalization error.

3.2 Relevance to the Air Force Mission and Potential Applications

The proposed function approximation approach can be used in Pulse Laser Deposition (PLD) application. PLD is an advanced process used to deposit a wide variety of thin coating for applications ranging from Air Force to civilian, superconductors to solid-lubricants. One of components of the PLD process modeling is focused on finding static nonlinear relationships. Our approach is perfect for this purpose.

The proposed dynamic updating approach can be used in Rugate filter processing application. Rugate filter processing is an advanced process used to deposit a variety of coating for applications for Air Force. The process needs in-situ monitoring and control. The rapid neural network learning model can be used as part of an intelligent hierarchical control system to guide the real-time feedback control of the process.

The regularization approach solves over-fitting problem for the neural network mapping. With regularization, the training is “immune” to the noise on the training data, which exist in most process data collection. The result gives us a very satisfactory generalization.

The proposed approach is a major potential strategy for accelerating materials design. The goal is to explore more efficient methods of organizing materials data using both supervised and unsupervised neural networks approach. Our approach can determine and predict ternary system compounding forming. Early, the entire research group that includes several scientists and engineers associated with Wright-Patterson AFB has discovered that the *Mendeleev number* could be used to predict, with 99% of accuracy, the occurrence of a compound for any multi-element (i.e., binary, ternary and etc.) materials systems. This discovery has save time and resource in exploring future materials systems. From this preliminary result, we have approximately narrowed down the search space of new materials. Furthermore, we extend the neural networks model to neuro-fuzzy model selection such that we can discovery most important features to predict the occurrence of a compound formation.

4. Personnel Supported

Financial support to these students

1. Gregory R. Schueller
2. Phil Edwards
3. William Lichtinger
4. Hang Nguyen

5. Publications

5.1 Journal Papers

1. C. L. P. Chen and J. Z. Wan, "A Rapid Learning and Dynamic Stepwise Updating Algorithm for Flat Neural Networks and its Application to Time-Series Prediction," *IEEE Trans. on Systems, Man and Cybernetics*, Vol. 29, No.1, pp. 62-72, 1999.
2. C. L. P. Chen, Y. Cao, and S. R. LeClair, "Materials structure-property prediction using a Self-Architecting Neural Network," *Journal of Alloys and Compounds*, 279, pp. 30-38, 1998.
3. C. L. P. Chen, S. R. LeClair, and Y-H. Pao, "An Incremental Adaptive Implementation of Functional-Link Process: for Function Approximation, Time-Series Prediction, and System Identification," *Neurocomputing, an International Journal*, Vol. 18, pp. 11-31, 1998.
4. C. L. P. Chen, "A Rapid Supervised Learning Neural Network for Function Interpolation and Approximation," *IEEE Trans. on Neural Networks*, Vol. 7, No. 5, pp. 1220-1230, 1996.
5. H. N. Al-Kamhawi, C. L. P. Chen, and S. R. LeClair, "Feature Sequencing in the Rapid Design System Using a Genetic Algorithm," *Journal of Intelligence Manufacturing*, Vol. 7, No. 1, pp. 55-67, 1996.
6. C. L. P. Chen and S. R. LeClair, "An Integration of Design and Manufacturing: Solving Setup Generation and Feature Sequencing Using Unsupervised Learning Approach," *Computer-Aided Design*, Vol. 26, No. 1, pp. 59-75, 1994.

5.2 Edited Books

1. C. Dagli, M. Akay, C. L. Philip Chen, B. R. Fernandez, and J. Ghosh, *Intelligent Engineering Systems Through Artificial Neural Networks: Fuzzy Logic and Evolutionary Programming*, ASME Press, 1995.
2. C. Dagli, M. Akay, C. L. Philip Chen, B. R. Fernandez, and J. Ghosh, *Smart Engineering System Design: Neural Networks, Fuzzy Logic, and Evolutionary Programming*, ASME Press, 1996.

5.3 Conference Papers

1. C. L. P. Chen and S. R. LeClair, "An Efficient Regularized Stepwise Learning Algorithms for Training Multi-output Orthogonal Functional Basis Neural Networks," *Proceedings of Artificial Neural Networks in Engineering*, Nov. 1-4, 1998, pp. 91-96.
2. C. L. P. Chen, Y. Cao, and S. R. LeClair, "Material Structure-Property Prediction using Orthogonal Functional Basis Neural Network," *Proceeding of Australasia Pacific Forum on Intelligent Processing and Manufacturing of Materials (IPMM)*, July, 14-17, 1997.
3. C. L. P. Chen, Y. Cao, and S. R. LeClair, "Orthogonal Functional Neural Network", *Proceeding of IEEE Int'l Conference on Neural Networks*, pp. 204-209, Huston, TX, June 9-12, 1997.
4. S. Ye and C. L. P. Chen, "Periodic Time-Series Analysis Using Neural Networks," *Proceeding of Artificial Neural Networks in Engineering*, pp. 719-724, 1996.
5. C. L. P. Chen and C-I. H. Chen, "Rapid Learning and Forecasting Using a Flat Neural Network for Circuit Design," *Proc. of 1996 IEEE International Symposium on Circuits and Systems*, pp. s18-s21, May 1996, Atlanta, GA.
6. C. L. P. Chen and S. R. LeClair, "A Real-time Stepwise Supervised Learning Algorithm for Time-Series Prediction and System Identification," *Proceeding of IEEE Int'l Conference on Neural Networks*, pp. 2009-2014, Washington, D.C., June 3-6, 1996.
7. C. L. P. Chen and J. Z. Wan, "Forecasting Time Series Using Instant Learning and Step-wise Updating," in *Proc. of Int'l Conference on Artificial Neural Networks in Engineering*, pp. 759-764, 1995.
8. C. L. P. Chen, S. R. LeClair, and Y-H. Pao, "A Rapid Supervised Learning Neural Network for Function Approximation and Time-Series

Prediction," in *Proceeding of Ohio Aerospace Institute Symposium*, pp. 23-34, 1995.

9. D. C. Moore, J. G. Jones, S. J. P. Laube, and C. L. P. Chen , "A Fast Learning Algorithm for Supervised-Learning Radial-Basis Function Neural Networks," *Ohio Aerospace Institute Symposium*, pp. 49-62, 1995.
10. I E. Ouais and C. L. P. Chen, "Instant Learning v/s Iterative Learning in a Flat Neural Network used in the Localization of Epileptogenic Foci," in *Proc. of World Congress on Neural Networks*, pp. Vol. II, pp. 776-780, Washington, D.C., 1995.
11. C. L. Philip Chen and S. R. LeClair, "An Efficient Supervised Learning Neural Network: An Architecture and Algorithm," *Proc. of Int'l Conference on Artificial Neural Networks in Engineering*, pp. 179-184, Nov. 13-16, 1994.

6. Interactions/Transactions

6.1 Participation/Presentations at Meetings, Conferences, Seminars

- Technical Committee, IEEE Int'l Conference on Robots and Systems, Oct. 16-21, 1999, Kyongij, Korea.
- Technical Committee of 1999 Int'l Conference on Neural Networks in Engineering, Nov. 7-Nov. 10, 1999, St. Louis, MO.
- Technical Committee, IEEE Int'l Conference on Robots and Systems, Oct. 12-16, 1998, Victoria, B.C., Canada.
- International Technical Committee (Industrial and Manufacturing Systems) of CESA'98 Computational Engineering in Systems Applications, France, April 1-4, 1998.
- Symposium Co-Chair of 1996 Adaptive Distributed Parallel Computing, Aug. 7-9, Dayton, Ohio.
- Technical Committee of 1996 IEEE Int'l Conference on Robotics and Automation, April 22-28, 1996, Minneapolis, MN.
- Conference Co-Chair of 1996 Int'l Conference on Neural Networks in Engineering, Nov. 10-Nov. 13, 1996-1998, St. Louis, MO.
- Conference Co-Chair of 1995 Int'l Conference on Neural Networks in Engineering, Nov. 12-Nov. 15, 1995, St. Louis, MO.
- Technical Committee of Ohio Aerospace Institute Neural Networks Symposium, Aug. 21-22, 1995, Athens, OH.
- Symposium Co-Organizer, 1994 Symposium of Applications of Innovative Knowledge Bases in Materials Design, Nov. 28-Dec. 2, 1994, Boston, MA.
- Tutorials Chair of 1994 IEEE Int'l Conf. on Neural Networks in IEEE World Congress on Computational Intelligence, June 26-July 2, 1994, Orlando, FL.

- Technical Committee of 1994 Int'l Conference on Neural Networks in IEEE World Congress on Computational Intelligence, June 26-July 2, 1994, Orlando, FL.
- Technical Committee of 1994 Int'l Conference on Neural Networks in Engineering, Nov. 13-Nov. 16, 1994, St. Louis, MO.
- Session Chairman in a paper session at the 1994 IEEE Int'l Conference on Systems, Man, and Cybernetics, Oct. 2-5, San Antonio, TX.

6.2 Consultative and Advisory Functions

Serve as a visiting research scientist with Materials Process Design Branch, Materials Directorate, Wright Laboratory (WL), Wright-Patterson Air Force Base (WPAFB), Dayton, Ohio.

The meeting is on a weekly base. The research subject is on "design self-learning and self-adaptive process system." The principal individual involved is the Technical Leader and Branch Chief, Dr. Steve R. LeClair.

7. New Discoveries, Inventions, or Patent Disclosures

- *Inductive-Deductive Process Design for Machined Parts*, Air Force Invention number 21134, U.S. Patent number 5485390, Jan, 1996, S. R. LeClair, Y. H. Pao, T. E. Westhoven, H. N. Al-Kamhawi, C. L. Philip Chen, A. G. Jackson, A. C. Chemaly.
- *Orthogonal Functional Basis Method for Function Approximation*, Air Force Invention No. D00211, Dec. 1996, Y. Cao, C. L. P. Chen, and S. R. LeClair.

8. Honors/Awards/Promotion

- Dr. Chen was promoted to the rank of Associate Professor in the year 1995.
- Research Excellent Faculty Award, College of Engineering and Computer Science, Wright State University, 1997.
- Senior Research Fellow, National Research Council, National Academy of Sciences/Engineering, 1997